

HPCx Service Report

August 2007

1 Introduction

This report covers the period from 0800 on 1 August 2007 to 0800 on 1 September 2007, a service month of 744 hours.

Overall utilisation of the main service fell back to just under 60%. Utilisation of the development service continues to be high, at nearly 93%. For the seventh month running, there were no SEV1 incidents.

2 Usage

2.1 Availability

Incidents

There were no incidents this month. Scheduled downtime was 4.3 hours for the maintenance session on the 8/8/2007.

The MTBF figures for this month were as follows:

| <i>SEV1</i> | <i>Incidents</i> | <i>MTBF</i> |
|----------------|------------------|-------------|
| IBM | 0.0 | ∞ |
| Site | 0.0 | ∞ |
| External | 0.0 | ∞ |
| <i>Overall</i> | 0.0 | ∞ |

Serviceability

| <i>Attribution</i> | <i>UDT</i> | <i>Serviceability</i> |
|--------------------|------------|-----------------------|
| IBM | 0:00 | 100.0 |
| Site | 0:00 | 100.0 |
| External | 0:00 | 100.0 |
| <i>Overall</i> | 0:00 | 100.0 |

2.2 CPU Usage by Consortium

Main Service

| <i>Consortium</i> | <i>CPU Hours (Parallel)</i> | <i>CPU Hours (Other)</i> | <i>AUs charged</i> | <i>%age of charged AUs</i> |
|--------------------|---------------------------------|------------------------------|------------------------|--------------------------------|
| e01 | 173485 | 159 | 817761 | 16.7% |
| e03 | 1 | 0 | 5 | 0.0% |
| e05 | 182161 | 511 | 867486 | 17.7% |
| e06 | 1019 | 0 | 4906 | 0.1% |
| e08 | 25343 | 0 | 122013 | 2.5% |
| e10 | 658 | 37 | 3347 | 0.1% |
| e11 | 8222 | 0 | 39586 | 0.8% |
| e17 | 266 | 3 | 1295 | 0.0% |
| e18 | 2451 | 0 | 11804 | 0.2% |
| e24 | 917 | 1 | 4417 | 0.1% |
| e26 | 1257 | 0 | 6052 | 0.1% |
| e33 | 129760 | 66 | 625043 | 12.7% |
| e35 | 212914 | 301 | 1026513 | 20.9% |
| e36 | 1372 | 0 | 5614 | 0.1% |
| e37 | 15032 | 0 | 72373 | 1.5% |
| e38 | 797 | 12 | 3896 | 0.1% |
| e39 | 17256 | 0 | 83076 | 1.7% |
| e41 | 6608 | 0 | 31813 | 0.6% |
| e42 | 44467 | 2 | 214094 | 4.4% |
| e44 | 1 | 0 | 4 | 0.0% |
| e46 | 1588 | 0 | 7643 | 0.2% |
| e49 | 4056 | 117 | 20092 | 0.4% |
| e50 | 2983 | 0 | 14363 | 0.3% |
| e53 | 6450 | 75 | 31417 | 0.6% |
| e60 | 6475 | 0 | 31171 | 0.6% |
| e61 | 593 | 0 | 2857 | 0.1% |
| <i>EPSRC Total</i> | 848188 | 1337 | 4058785 | 82.7% |

| | | | | |
|-------------------|--------|-----|--------|-------|
| n01 | 261 | 0 | 1255 | 0.0% |
| n02 | 111832 | 8 | 538447 | 11.0% |
| n03 | 24193 | 397 | 118391 | 2.4% |
| n04 | 22925 | 35 | 110541 | 2.3% |
| <i>NERC Total</i> | 159211 | 441 | 768634 | 15.7% |

| | | | | |
|--------------------|----|---|-----|------|
| p01 | 23 | 1 | 117 | 0.0% |
| <i>PPARC Total</i> | 23 | 1 | 117 | 0.0% |

| | | | | |
|--------------------|-----|---|------|------|
| c01 | 450 | 0 | 2168 | 0.0% |
| <i>CCLRC Total</i> | 450 | 0 | 2168 | 0.0% |

| | | | | |
|--------------------|------|---|-------|------|
| b08 | 7561 | 0 | 36404 | 0.7% |
| <i>BBSRC Total</i> | 7561 | 0 | 36404 | 0.7% |

| | | | | |
|-----------------------|----|---|----|------|
| x01 | 20 | 0 | 98 | 0.0% |
| <i>External Total</i> | 20 | 0 | 98 | 0.0% |

| | | | | |
|-------------------|------|----|-------|------|
| z001 | 6984 | 9 | 33667 | 0.7% |
| z004 | 1759 | 13 | 8529 | 0.2% |
| z06 | 4 | 0 | 19 | 0.0% |
| <i>HPCx Total</i> | 8747 | 25 | 42229 | 0.9% |

Development Service

| <i>Consortium</i> | <i>CPU Hours (Parallel)</i> | <i>CPU Hours (Other)</i> | <i>AUs charged</i> | <i>%age of charged AUs</i> |
|-------------------|---------------------------------|------------------------------|------------------------|--------------------------------|
| n01 | 0 | 0 | 0 | 0.0% |
| n02 | 130655 | 422 | 631063 | 99.4% |
| n03 | 802 | 0 | 3859 | 0.6% |
| <i>NERC Total</i> | 131457 | 422 | 634922 | 100.0% |

2.3 CPU Usage by Job Type

The figures for *Raw AUs* given here show the number of AUs actually supplied by the system to users' jobs.

Main service

| <i>Number of processors</i> | <i>Raw AUs</i> | <i>%age</i> | <i>Number of jobs</i> |
|-----------------------------|----------------|-------------|-----------------------|
| ≤32 | 553509 | 11.2% | 3843 |
| 33–64 | 680738 | 13.8% | 687 |
| 65–128 | 1268967 | 25.7% | 840 |
| 129–256 | 1714194 | 34.8% | 660 |
| 257–512 | 695258 | 14.1% | 137 |
| 513–1024 | 15108 | 0.3% | 31 |
| >1024 | 3187 | 0.1% | 8 |

Overall utilisation of the main service was 58.5%. Capability usage was 14.5% of the total.

Development Service

| <i>Number of processors</i> | <i>Raw AUs</i> | <i>%age</i> | <i>Number of jobs</i> |
|-----------------------------|----------------|-------------|-----------------------|
| ≤32 | 630789 | 99.7% | 6251 |
| 33–64 | 2103 | 0.3% | 24 |

Overall utilisation of the development service was 92.6%.

2.4 Slowdown and Job Wait Times

Slowdowns

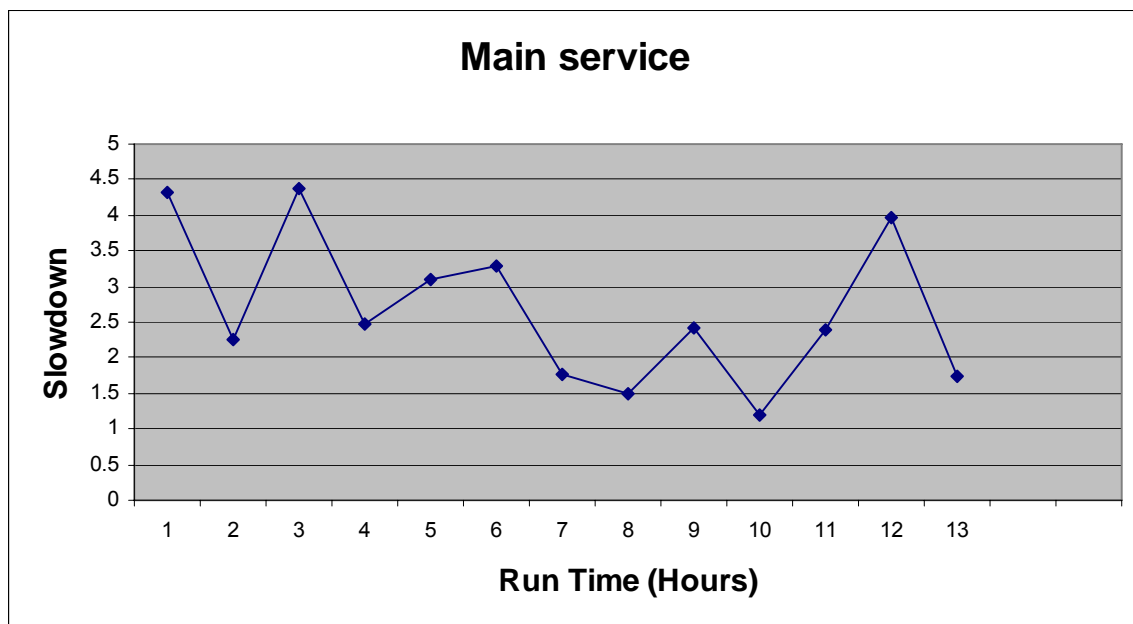
Slowdown is a widely used measure of the relative wait times of different classes of jobs. It is defined as:

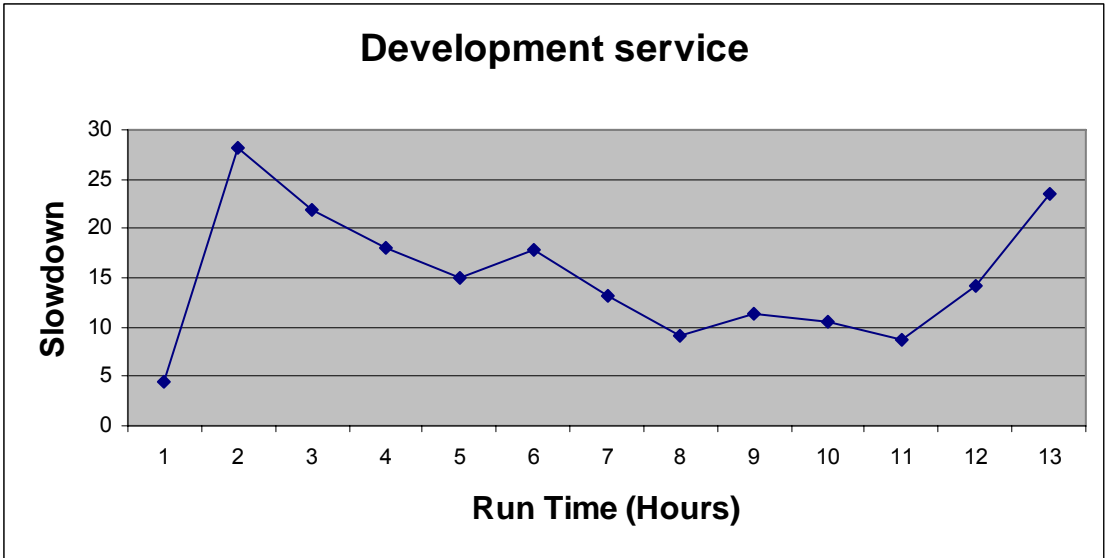
$$\text{Slowdown} = (\text{job run time} + \text{job wait time}) / (\text{job run time})$$

Slowdowns of less than around 10 are usually regarded as reasonable.

Slowdowns by runtime

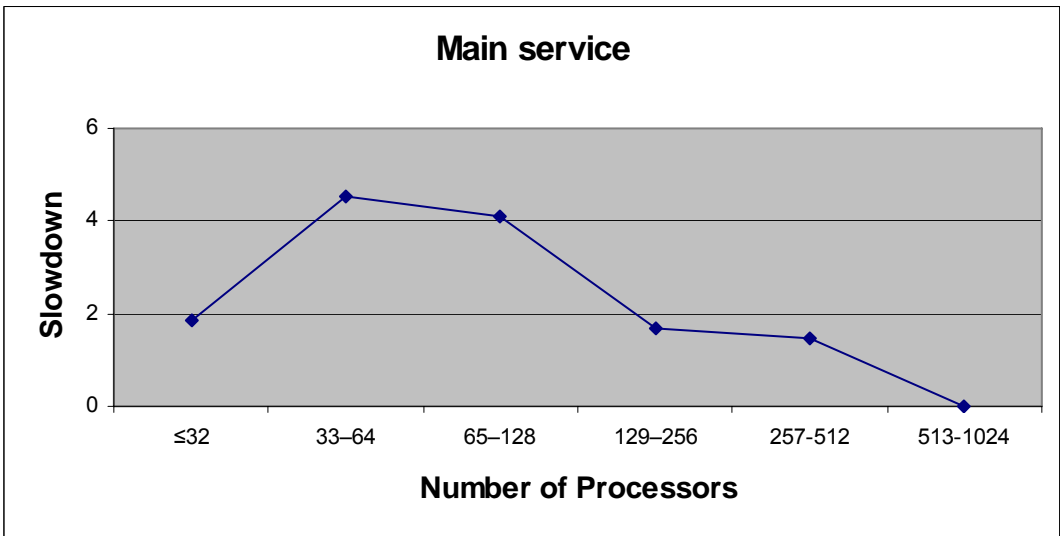
The following graphs show the slowdowns recorded for jobs of differing run times, ignoring those which ran for less than 5 minutes.

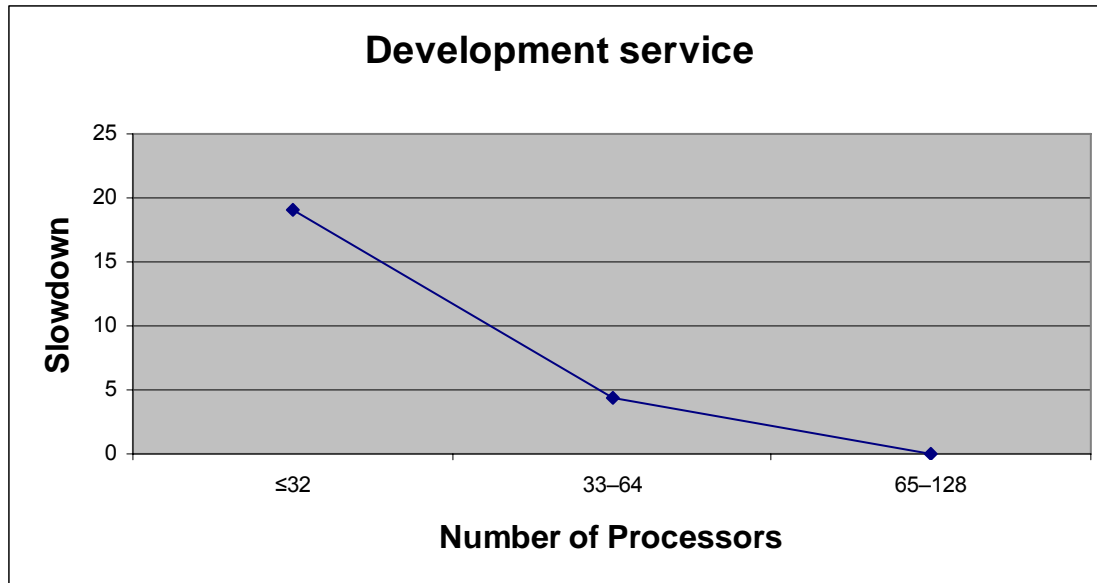




Slowdowns by number of processors

In the graphs below, we plot the slowdown figures against the number of processors used. Only jobs which ran for more than 1 hour are included.





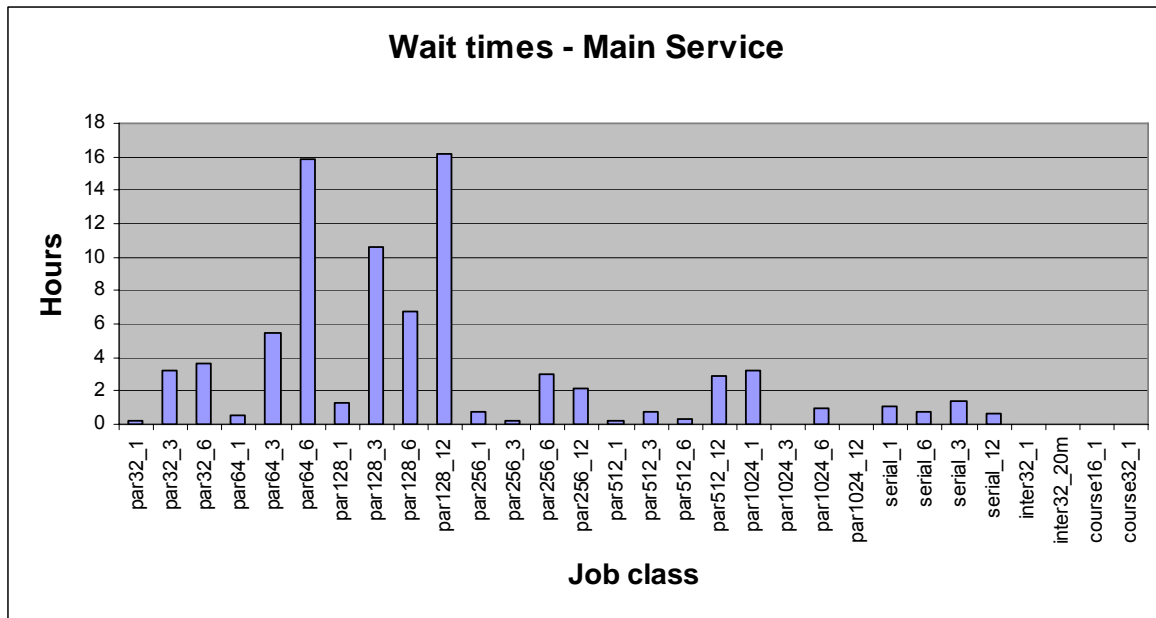
On both services, slowdowns are currently generally satisfactory.

Job wait times – main service

The following table and graph shows the average wait time (in hours) for each class of job on the main service.

| <i>Job Class</i> | <i>Category</i> | <i>Maximum Number of CPUs</i> | <i>Maximum Job length</i> | <i>Average wait time</i> | <i>Number of Jobs</i> |
|------------------|-----------------|-------------------------------|---------------------------|--------------------------|-----------------------|
| par32_1 | parallel | 32 | 1 | 0.2 | 2642 |
| par32_3 | parallel | 32 | 3 | 3.2 | 92 |
| par32_6 | parallel | 32 | 6 | 3.6 | 1109 |
| par64_1 | parallel | 64 | 1 | 0.6 | 163 |
| par64_3 | parallel | 64 | 3 | 5.5 | 25 |
| par64_6 | parallel | 64 | 6 | 15.9 | 499 |
| par128_1 | parallel | 128 | 1 | 1.3 | 444 |
| par128_3 | parallel | 128 | 3 | 10.6 | 168 |
| par128_6 | parallel | 128 | 6 | 6.8 | 41 |
| par128_12 | parallel | 128 | 12 | 16.2 | 187 |
| par256_1 | parallel | 256 | 1 | 0.7 | 193 |
| par256_3 | parallel | 256 | 3 | 0.2 | 91 |
| par256_6 | parallel | 256 | 6 | 3.0 | 135 |
| par256_12 | parallel | 256 | 12 | 2.2 | 241 |
| par512_1 | parallel | 512 | 1 | 0.2 | 55 |
| par512_3 | parallel | 512 | 3 | 0.8 | 13 |
| par512_6 | parallel | 512 | 6 | 0.4 | 31 |
| par512_12 | parallel | 512 | 12 | 2.9 | 38 |

| | | | | | |
|-------------|-------------|------|----|-----|------|
| par1024_1 | parallel | 1024 | 1 | 3.2 | 26 |
| par1024_3 | parallel | 1024 | 3 | 0.0 | 0 |
| par1024_6 | parallel | 1024 | 6 | 1.0 | 5 |
| par1024_12 | parallel | 1024 | 12 | 0.0 | 0 |
| serial_1 | serial | 1 | 1 | 1.1 | 3096 |
| serial_6 | serial | 1 | 6 | 0.7 | 297 |
| serial_3 | serial | 1 | 3 | 1.4 | 59 |
| serial_12 | serial | 1 | 12 | 0.7 | 24 |
| inter32_1 | interactive | 32 | 1 | 0.0 | 0 |
| inter32_20m | interactive | 32 | 1 | 0.0 | 967 |
| course16_1 | interactive | 16 | 1 | 0.0 | 0 |
| course32_1 | parallel | 32 | 1 | 0.0 | 0 |

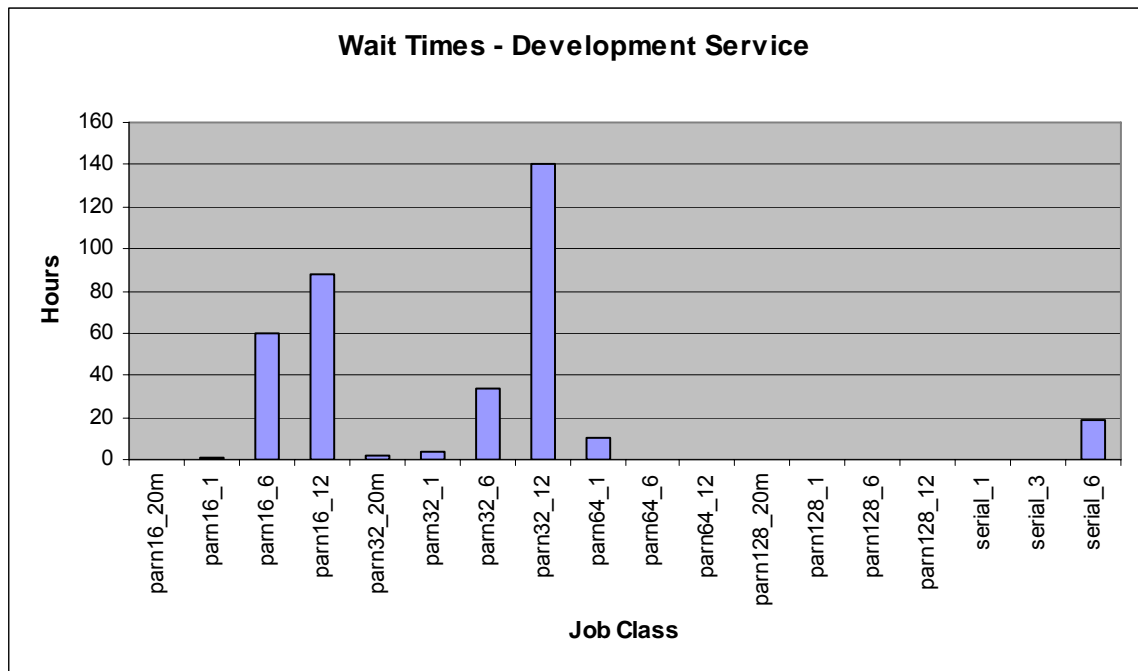


Job wait times – development service

As we noted last month, wait times on the development service have lengthened to some degree, as a result of the high utilisation of the service (almost 93%).

| Job Class | Category | Maximum Number of CPUs | Maximum Job length | Average wait time | Number of Jobs |
|------------|----------|------------------------|--------------------|-------------------|----------------|
| parn16_20m | parallel | 16 | 20 mins | 0.2 | 1771 |
| parn16_1 | parallel | 16 | 1 hour | 1.4 | 2187 |
| parn16_6 | parallel | 16 | 6 hours | 59.8 | 268 |
| parn16_12 | parallel | 16 | 12 hours | 88.0 | 263 |
| parn32_20m | parallel | 32 | 20 mins | 1.4 | 465 |
| parn32_1 | parallel | 32 | 1 hour | 3.7 | 1192 |
| parn32_6 | parallel | 32 | 6 hours | 33.9 | 10 |
| parn32_12 | parallel | 32 | 12 hours | 140.7 | 95 |

| | | | | | |
|-------------|----------|-----|----------|------|------|
| parn64_1 | parallel | 64 | 1 hour | 9.8 | 23 |
| parn64_6 | parallel | 64 | 6 hours | 0.0 | 0 |
| parn64_12 | parallel | 64 | 12 hours | 0.0 | 0 |
| parn128_20m | parallel | 128 | 20 mins | 0.0 | 0 |
| parn128_1 | parallel | 128 | 1 hour | 0.0 | 0 |
| parn128_6 | parallel | 128 | 6 hours | 0.0 | 0 |
| parn128_12 | parallel | 128 | 12 hours | 0.0 | 0 |
| serial_1 | serial | 1 | 1 hour | 0.1 | 6537 |
| serial_3 | serial | 1 | 12 hours | 0.0 | 145 |
| serial_6 | serial | 1 | 12 hours | 19.1 | 170 |



2.5 Disk Occupancy

Home Space

Home space is the part of the disk space that is regularly backed up.

| | | |
|-----|---------|---------|
| b02 | 34,058 | 50,000 |
| b03 | 52,711 | 50,000 |
| b08 | 21,036 | 50,000 |
| c01 | 163,367 | 300,000 |
| e01 | 192,009 | 199,995 |
| e03 | 62,517 | 225,012 |
| e05 | 376,297 | 665,550 |
| e06 | 288,513 | 300,000 |
| e08 | 93,580 | 100,000 |
| e10 | 98,523 | 150,000 |
| e11 | 42,777 | 100,000 |
| e14 | 74,309 | 100,000 |
| e15 | 40,730 | 50,000 |
| e16 | 133 | 20,000 |
| e17 | 44,927 | 50,000 |
| e18 | 37,754 | 40,000 |
| e19 | 1,417 | 40,000 |
| e20 | 58,105 | 60,000 |
| e21 | 1,521 | 50,000 |
| e22 | 5,268 | 10,000 |
| e23 | 9,733 | 50,000 |
| e24 | 63,744 | 394,376 |
| e25 | 14,459 | 50,000 |
| e26 | 17,033 | 20,000 |
| e27 | 19,054 | 20,000 |
| e29 | 23,455 | 50,000 |
| e31 | 35,459 | 50,000 |
| e32 | 47,110 | 50,000 |
| e33 | 22,993 | 50,000 |
| e35 | 65,216 | 100,000 |
| e36 | 49,109 | 100,000 |
| e37 | 129,430 | 204,800 |
| e38 | 45,722 | 50,000 |
| e39 | 105,857 | 150,000 |
| e40 | 18,109 | 50,000 |
| e41 | 1,532 | 100,000 |
| e42 | 65,381 | 100,000 |
| e44 | 19 | 50,000 |
| e45 | 43,936 | 50,000 |
| e46 | 7,105 | 50,000 |

| | | |
|------|---------|---------|
| e48 | 5 | 50,000 |
| e49 | 39,800 | 50,000 |
| e50 | 3,565 | 13,000 |
| e51 | 5,181 | 50,000 |
| e52 | 11 | 50,000 |
| e53 | 13,420 | 50,000 |
| e54 | 46,526 | 50,000 |
| e55 | 1,664 | 50,000 |
| e56 | 47,509 | 50,000 |
| e58 | 19,291 | 100,000 |
| e59 | 1,348 | 100,000 |
| e60 | 17,396 | 50,000 |
| e61 | 19,263 | 50,000 |
| e62 | 2,255 | 50,000 |
| n01 | 107,056 | 250,000 |
| n02 | 166,728 | 299,900 |
| n03 | 98,558 | 100,000 |
| n04 | 192,278 | 299,999 |
| p01 | 52,492 | 200,000 |
| x01 | 49,190 | 50,000 |
| x02 | 8,746 | 20,000 |
| x03 | 4,227 | 50,000 |
| z001 | 516,686 | 600,000 |
| z002 | 89,501 | 124,000 |
| z004 | 95,644 | 100,000 |
| z05 | 4,188 | 30,000 |
| z06 | 64,758 | 75,000 |
| z07 | 40,698 | 50,000 |
| z10 | 1,980 | 50,000 |

Workspace

| <i>Consortium</i> | <i>Disc Occupancy (Mb)</i> | <i>Disc Quota (Mb)</i> |
|-------------------|----------------------------|------------------------|
| b02 | 15 | 1,025 |
| b03 | 47,908 | 100,000 |
| b08 | 5,100 | 50,000 |
| c01 | 89,093 | 100,000 |
| e01 | 1,335,292 | 1,349,995 |
| e03 | 10 | 500,000 |
| e05 | 441,656 | 666,005 |
| e06 | 367,943 | 400,000 |
| e08 | 141 | 5,000 |
| e10 | 346,587 | 400,000 |
| e11 | 48,527 | 100,000 |
| e14 | 121,478 | 250,000 |
| e15 | 36,691 | 100,000 |

| | | |
|------|-----------|-----------|
| e17 | 134,939 | 200,000 |
| e18 | 51,245 | 80,000 |
| e19 | 169,244 | 200,000 |
| e20 | 949,980 | 1,000,000 |
| e21 | 1 | 100,000 |
| e23 | 38,039 | 100,000 |
| e24 | 1 | 2,800,000 |
| e25 | 142,925 | 150,000 |
| e27 | 2,760 | 40,000 |
| e29 | 7 | 9,800 |
| e31 | 93,144 | 100,000 |
| e32 | 99,998 | 100,000 |
| e33 | 50,679 | 100,000 |
| e35 | 33,762 | 200,000 |
| e36 | 50,770 | 200,000 |
| e37 | 254,231 | 307,200 |
| e40 | 1 | 100,000 |
| e41 | 169,046 | 200,000 |
| e42 | 353,110 | 400,000 |
| e48 | 95,722 | 200,000 |
| e49 | 38,704 | 50,000 |
| e50 | 180,916 | 100,000 |
| e53 | 1,797 | 150,000 |
| e56 | 99,999 | 100,000 |
| e61 | 24,578 | 100,000 |
| e62 | 3,816 | 200,000 |
| e63 | 405 | 200,000 |
| n01 | 243,073 | 800,000 |
| n02 | 7,059,626 | 8,499,904 |
| n03 | 24,200 | 81,002 |
| n04 | 581,728 | 750,000 |
| p01 | 41,764 | 50,000 |
| x01 | 158,299 | 160,000 |
| x03 | 178 | 50,000 |
| z001 | 530,916 | 600,000 |
| z002 | 1,617 | 770 |
| z004 | 17,601 | 25,000 |
| z05 | 4,740 | 20,000 |
| z06 | 57,096 | 100,000 |
| z07 | 4 | 20,000 |

Development service space

This is the disk space reserved for users of the development service.

| <i>Consortium</i> | <i>Disc Occupancy (Mb)</i> | <i>Disc Quota (Mb)</i> |
|-------------------|----------------------------|------------------------|
| n02 | 6,840,331.50 | 9,499,003 |
| n04 | 6,468.20 | 526,899 |

2.6 Tape Archive

| <i>Consortium</i> | <i>Usage (Tapes)</i> | <i>Quota (Tapes)</i> | <i>Files</i> | <i>Data (Gb)</i> |
|-------------------|----------------------|----------------------|--------------|------------------|
| c01 | 2 | 2 | 7,231 | 65 |
| e01 | 70 | 70 | 429,774 | 6,339 |
| e03 | 5 | 5 | 18,797 | 429 |
| e14 | 10 | 10 | 391,623 | 595 |
| e15 | 1 | 3 | 26 | 6 |
| e24 | 10 | 10 | 7,785 | 803 |
| e26 | 2 | 2 | 545 | 27 |
| e42 | 10 | 10 | 29,481 | 447 |
| n01 | 313 | 325 | 35,162 | 33,686 |
| n02 | 579 | 585 | 691,688 | 64,804 |
| n04 | 28 | 30 | 116,775 | 3,740 |
| z001 | 7 | 10 | 11,045 | 67 |
| z002 | 2 | 3 | 5,801 | 15 |
| z06 | 1 | 3 | 833 | 68 |

Note that a tape is counted in the *Usage* column even if it is only partly occupied.

3 Support

3.1 Helpdesk

Classifications

| <i>Service metric</i> | <i>Number</i> | <i>% of all</i> |
|-----------------------|---------------|-----------------|
| Administrative | 30 | 47.6% |
| Technical | 27 | 42.9% |
| In-depth | 5 | 7.9% |
| Technical assessment | 1 | 1.6% |
| PMR | 0 | 0.0% |
| <i>Total</i> | 63 | 100.0% |

The *PMR* service metric includes in-depth queries that result in Problem Management Reports for IBM. The *Technical Assessment* metric has been added since technical assessments are now being handled through the helpdesk, for compatibility with the HECToR procedure.

In place of the former *Service Area* information we shall supply a breakdown of queries by subject category.

| <i>Category</i> | <i>Number</i> | <i>% of all</i> |
|-------------------------------|---------------|-----------------|
| Disks, tapes, resources | 15 | 23.8% |
| Compilers and system software | 10 | 15.9% |
| 3rd party software | 10 | 15.9% |
| Login, passwords, ssh | 6 | 9.5% |
| Batch system and queues | 6 | 9.5% |
| SAFE | 5 | 7.9% |
| Other | 3 | 4.8% |
| Access to HPCx | 3 | 4.8% |
| None | 2 | 3.2% |
| User programs | 1 | 1.6% |
| User behaviour | 1 | 1.6% |
| Performance and scaling | 1 | 1.6% |
| <i>Total</i> | 63 | 100.0% |

Performance

| <i>Metric</i> | <i>Achieved</i> | <i>Total</i> | <i>Fraction</i> | <i>Target</i> |
|-----------------------------------|-----------------|--------------|-----------------|---------------|
| Administrative queries - two days | 25 | 30 | 83% | 97% |
| All queries - three days | 55 | 57 | 96% | 97% |
| All queries - one day | 33 | 57 | 58% | 75% |

Query handlers

| <i>Handler</i> | <i>Technical</i> | <i>In-depth</i> | <i>Admin</i> | <i>PMR</i> | <i>Technical assessment</i> |
|----------------|------------------|-----------------|--------------|------------|-----------------------------|
| Sysadm | 15 | 1 | 12 | 0 | 0 |
| DL | 4 | 3 | 1 | 0 | 0 |
| EPCC | 8 | 1 | 17 | 0 | 1 |

3.2 Training done

There were no training courses this month.

4 Staffing

4.1 Science Support Staffing

Daresbury Laboratory

| <i>Name</i> | <i>Days</i> |
|--------------|-------------|
| Ashworth | 10.0 |
| Blake | 2.2 |
| Bush | 12.0 |
| Johnstone | 13.2 |
| Jones | 3.3 |
| Plummer | 11.0 |
| Sunderland | 22.0 |
| Todorov | 6.4 |
| Total (Days) | 80.1 |
| FTEs | 4.5 |

EPCC

| <i>Name</i> | <i>Days</i> |
|---------------------|-------------|
| Simpson | 20.6 |
| Booth | 13.2 |
| Henty | 10.9 |
| Bull | 6.3 |
| Fisher | 4.0 |
| Hein | 10.4 |
| Jackson | 4.1 |
| Reid | 20.7 |
| Stratford | 0.9 |
| Trew | 4.3 |
| Gray | 12.3 |
| D'Mellow | 10.0 |
| Hill | 7.0 |
| Johnson | 0.5 |
| Maynard | 3.1 |
| Weiland | 27.6 |
| Other staff | 20.6 |
| <i>Total (Days)</i> | 200.0 |
| <i>FTEs</i> | 11.3 |

Overall Levels

| | <i>FTEs</i> |
|-------|-------------|
| DL | 4.5 |
| EPCC | 11.3 |
| Total | 15.8 |

4.2 Systems Staffing

| <i>Name</i> | <i>Days</i> |
|---------------------|-------------|
| Andrews | 9.4 |
| Brown | 12.0 |
| Fisher | 12.0 |
| Georgeson | 15.3 |
| Franks | 10.8 |
| Jones | 0.8 |
| BITD | 22.0 |
| Morey | 10.0 |
| Nazarova | 8.9 |
| Collard | 3.83 |
| Kalavsky | 4.4 |
| Andrews | 9.4 |
| <i>Total (days)</i> | 109.4 |
| <i>FTEs</i> | 6.2 |

Note: BITD covers a range of bookings from a support department who provide approximately 1 FTE to support computer room operations, electrical and mechanical site services and networking and security. Roughly a dozen staff charge time to the project in amounts which vary from month to month. We believe that it adds no value to report these individual bookings although a full listing can be provided annually if required.

5 Summary of Performance Metrics

| <i>Metric</i> | <i>TSL</i> | <i>FSL</i> | <i>Monthly Measurement</i> |
|---|------------|------------|----------------------------|
| Technology serviceability | 80% | 99.2% | 100.0% |
| Technology MTBF (hours) | 200 | 300 | ∞ |
| Number of AV FTEs | 7.5 | 10 | 15.8 |
| Number of training days per month | 20/12 | 25/12 | 13/8 |
| Non in-depth queries resolved within 3 days | 85% | 97% | 96.5% |
| Number of A&M FTEs | 3.75 | 5.75 | 6.2 |
| A&M serviceability | 80% | 99.6% | 100.0% |

Appendix A: Incident Severity Levels

SEV 1 — anything that comprises a FAILURE as defined in the contract with EPSRC.

SEV 2 — NON-FATAL incidents that typically cause immediate termination of a user application, but not the entire user service.

The service may be so degraded (or liable to collapse completely) that a controlled, but unplanned (and often very short-notice) shutdown is required or unplanned downtime subsequent to the next planned reload is necessary.

This category includes unrecovered disc errors where damage to filesystems may occur if the service was allowed to continue in operation; incidents when although the service can continue in operation in a degraded state until the next reload, downtime at less than 24 hours notice is required to fix or investigate the problem; and incidents whereby the throughput of user work is affected (typically by the unrecovered disabling of a portion of the system) even though no subsequent unplanned downtime results.

SEV 3 — NON-FATAL incidents that typically cause immediate termination of a user application, but the service is able to continue in operation until the next planned reload or re-configuration.

SEV 4 — NON-FATAL recoverable incidents that typically include the loss of a storage device, or a peripheral component, but the service is able to continue in operation largely unaffected, and typically the component may be replaced without any future loss of service.

Appendix B: Projects

B.1 Current Projects

EPSRC Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|---|---------------------------|
| e01 | 1 | UK Turbulence Consortium | Dr Gary Coleman |
| e05 | 1 | Materials Chemistry using Terascaling Computing | Prof Richard Catlow |
| e06 | 1 | UK Car-Parrinello Consortium | Prof Paul Madden |
| e08 | 2 | Organic Solid State | Prof Sarah Price |
| e10 | 1 | Reality Grid | Prof Peter Coveney |
| e11 | 1 | Bond making and breaking at surfaces | Prof Sir David A King |
| e14 | 1 | Blade and Cavity Noise | Prof Neil Sandham |
| e15 | 2 | CSAR/HPCx Collaboration | Dr Mike Pettipher |
| e16 | 1 | Cardiac virtual tissues | Prof Arun V Holden |
| e17 | 1 | Integrative Biology | Dr David Gavaghan |
| e18 | 1 | DARP: Highly swept leading edge separations | Prof Michael A Leschziner |
| e19 | 1 | Edinburgh Soft Matter and Statistical Physics Group | Prof Michael E Cates |
| e20 | 1 | UK Applied Aerodynamics Consortium | Dr Ken Badcock |
| e21 | 1 | Intrinsic Parameter Fluctuations in Decanometer MOSFETs | Prof Asen M Asenov |
| e22 | 1 | Preconditioners for finite element problems | Prof David J Silvester |
| e23 | 1 | Exploitation of Switched Lightpaths for e-Science Applications | Prof Peter Clarke |
| e24 | 1 | DEISA - Distributed European Infrastructure for Supercomputing Applications | Dr David Henty |
| e25 | 1 | Turbulent vortex motion in stratified flows | Dr Gary Coleman |
| e26 | 1 | Simulation of Radioprobing | Dr Charlie Laughton |
| e27 | 1 | SPICE | Prof Peter V Coveney |
| e29 | 1 | Free-surface-piercing circular cylinders | Dr Eldad Avital |

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| e30 | 1 | Metal/Oxide Interfaces at the Atomic Level | Dr Nora de Leeuw |
| e31 | 1 | Lateral Straining of Wall-Bounded Turbulence | Dr Gary N Coleman |
| e32 | 1 | Rapid Prototyping of Usable Grid Middleware | Prof Peter V Coveney |
| e33 | 1 | Engineering Functional Coatings | Prof Roger Smith |
| e34 | 1 | Dissolution of Bioactive Phosphate Glasses | Dr N de Leeuw |
| e35 | 1 | Non-adiabatic processes | Dr T Todorov |
| e36 | 1 | Jets in Cross-Flow | Dr Y Yao |
| e37 | 1 | LESUK_3 | Prof J J McGuirk |
| e38 | 1 | Viscoelastic deformation in 3D non-linear media | Prof Greg A Houseman |
| e39 | 1 | The Supergen 5 biological fuel cells consortium | Prof FA Armstrong |
| e40 | 1 | Computational Quantum Many-Body Theory | Prof R Needs |
| e41 | 1 | Flow in Weapon Bays | Dr George N Barakos |
| e42 | 1 | Computational Combustion for Engineering Applications | Prof K Luo |
| e44 | 1 | Extreme Wave Loading on Offshore Wave Energy Devices | Dr Deborah Greaves |
| e45 | 1 | Metals under extreme conditions | Prof Mike Gillan |
| e46 | 1 | Advanced materials with complex architectures | Dr Paul Mummery |
| e47 | 1 | Parallel stochastic analysis for geo-engineering | Dr Michael A. Hicks |
| e48 | 1 | Organised structure in turbulent flows | Prof Sergei Chernyshenko |
| e49 | 1 | Integrated Programme of Research in Aeronautical Engineering | Prof Michael Leschziner |
| e50 | 1 | Biological interface with materials | Prof John Harding |
| e51 | 1 | Super-computing data mining | Dr Mike Pettipher |
| e52 | 1 | Spacecraft force modelling | Dr M Ziebart |
| e53 | 1 | Large-scale communication networks | Prof J M Pitts |
| e54 | 1 | Free surface simulation of waves overtopping during storms | Dr D M Ingram |

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| e55 | 1 | High-Reynolds-Number Near-Wall Flows | Prof Michael Leschziner |
| e56 | 1 | Infectious disease threats | Dr Iain Barrass |
| e57 | 1 | Triplex DNA Structures | Dr Hooshang Nikjoo |
| e58 | 1 | Quantum Simulations for Chemical Biology | Dr Carmen Domene |
| e59 | 1 | Turbulence in breaking gravity waves | Prof Ian Castro |
| e60 | 1 | Device Electronics Based on nanoWires and NanoTubes | Dr Merlyne M de Souza |
| e61 | 1 | Enhancement of droplet concentrations in clouds | Dr Alan A M Gadian |
| e62 | 1 | Low Voltage Defibrillation | Dr Vadim Biktashev |

PPARC Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|---------------------------------|-------------------|
| p01 | 1 | Atomic Physics and Astrophysics | Prof Alan Hibbert |

NERC Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|--|--------------------|
| n01 | 1 | Large-Scale Long-Term Ocean Circulation | Dr David Webb |
| n02 | 1 | NCAS | Prof Alan J Thorpe |
| n03 | 1 | Computational Mineral Physics Consortium | Dr John Brodholt |
| n04 | 1 | Shelf Seas Consortium | Dr Roger Proctor |

BBSRC Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|----------------------------|------------------------|
| b02 | 1 | Modelling enzyme catalysis | Dr Adrian J Mulholland |
| b08 | 1 | IntBioSim | Prof M S Sansom |

CCLRC Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|--|--------------------|
| c01 | 1 | Daresbury Laboratory Facilities Agreement Consortium | Dr Richard J Blake |

Externally-funded Projects

| <i>Code</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|---------------------|
| x01 | HPC-Europa | Dr Judy Hardy |
| x03 | IBM | Mr Derrick J Byford |

HPCx Projects

| <i>Code</i> | <i>Title</i> | <i>PI</i> |
|-------------|------------------------|--------------------|
| z001 | HPCx Support | Dr Alan Simpson |
| z002 | Systems and Operations | Mr Mike Brown |
| z003 | Test Project | Dr Denis Nicole |
| z004 | HPCx Training | Dr David Henty |
| z05 | Outreach Projects | Dr Richard Blake |
| z06 | Application Porting | Dr David Henty |
| z07 | Package Installation | Dr Mike Ashworth |
| z10 | Globus | Dr Stephen P Booth |

B.2 Former Projects

| <i>Code</i> | <i>Class</i> | <i>Title</i> | <i>PI</i> |
|-------------|--------------|--|------------------------|
| b01 | 2 | Quantum Chemistry Studies of the Rusticyanin Protein Crystal | Prof Samar Hasnain |
| b03 | 1 | Towards a virtual outer membrane | Prof Mark S Sansom |
| b04 | 1 | Life sciences software development | Dr Jo L Dicks |
| b05 | 1 | Virtual forced evolution of catalytic transition metal complexes | Dr Marcus Durrant |
| b06 | 2 | Biomolecular computational chemistry | Prof Jonathan D Hirst |
| e02 | 1 | Ab-initio simulation of covalently bonded materials | Dr Patrick Briddon |
| e03 | 1 | Multi-photon, electron collisions and BEC HPC consortium | Prof Ken Taylor |
| e04 | 1 | Chemreact Computing Consortium | Prof Jonathon Tennyson |
| e07 | 2 | Turbulent Plasma Transport in Tokamaks | Dr Colin M Roach |
| e09 | 2 | Molecular Properties and their Geometry | Dr Mark R Wilson |

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|-----|---|--|---------------------|
| e12 | 1 | Parallel programs for the simulation of complex fluids | Dr Richard J Blake |
| e13 | 1 | TeraGyroid project | Mr Mark Westwood |
| e28 | 1 | Towards the Dynome | Dr Jonathan W Essex |
| z09 | | HECToR Benchmarking | Dr Edward Smyth |
| x02 | | OHM Ltd | Dr Lucy MacGregor |
| n05 | 2 | Non-linear Wave-particle Instabilities in Plasmas | Dr Mervyn Freeman |